PROJECT NUMBER: 1754
PROJECT TITLE: Spectroscopic Studies of Tobacco and Smoke Components
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PERIOD COVERED: June, 1988

SOLID STATE NMR OF TOBACCO COMPONENTS

A. **Objective**: Determine the composition and structure of tobacco cell wall biopolymers (J. Wooten).

B. **Results**: Stem tissue L. leucocephala that was fed β-^{13}C ferulic acid for extended periods during its growth was examined by ^{13}C CP/MAS NMR for ^{13}C labelled carbons in the cell wall lignin. The ^{13}C incorporation was insufficient to unambiguously draw conclusions about the lignin bonding patterns, in part because of negative signals in the difference spectrum between ^{13}C and ^{12}C labelled plant tissue. The negative signals are an indication that the plant metabolism in the two sets of plants was not identical. This difficulty must be resolved before low levels of ^{13}C labels can be detected.

A. **Objective**: Determine the composition of the base gum in "Chewbacco".

B. **Results**: The outside coating of "Chewbacco" was removed and the interior base gum was examined intact by ^{13}C CP/MAS NMR and single pulse MAS NMR. Cross polarization (CP) is effective for detecting rigid (hard) components while the single pulse method detects components that are very much more mobile (soft). The two types of spectra were very different, indicating a mixture of soft and hard components in the gum. The signals have been only partially assigned. The soft component contains signals that match polyvinyl acetate and a signal that corresponds to polymethylene chains, possibly polyisobutylene rubber. Weak aromatic signals appear which may be nicotine in the the soft gum portions. Several signals corresponding to hydroxyl bearing carbons appear in both the hard and soft components. These signals may result partially from sorbitol, which has been identified in the water soluble portion of "Chewbacco", but appear to be primarily an unidentified polysaccharide polymer. A signal from polymethylene chains also appears in the hard component spectrum.

C. **Plans**: Solution NMR spectra will be obtained and compared with the solid state results. The spectra will be interpreted on the basis of the previously reported compositions of chewing gum base.

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